Potential optimization for the calculation of shocked liquid nitromethane properties

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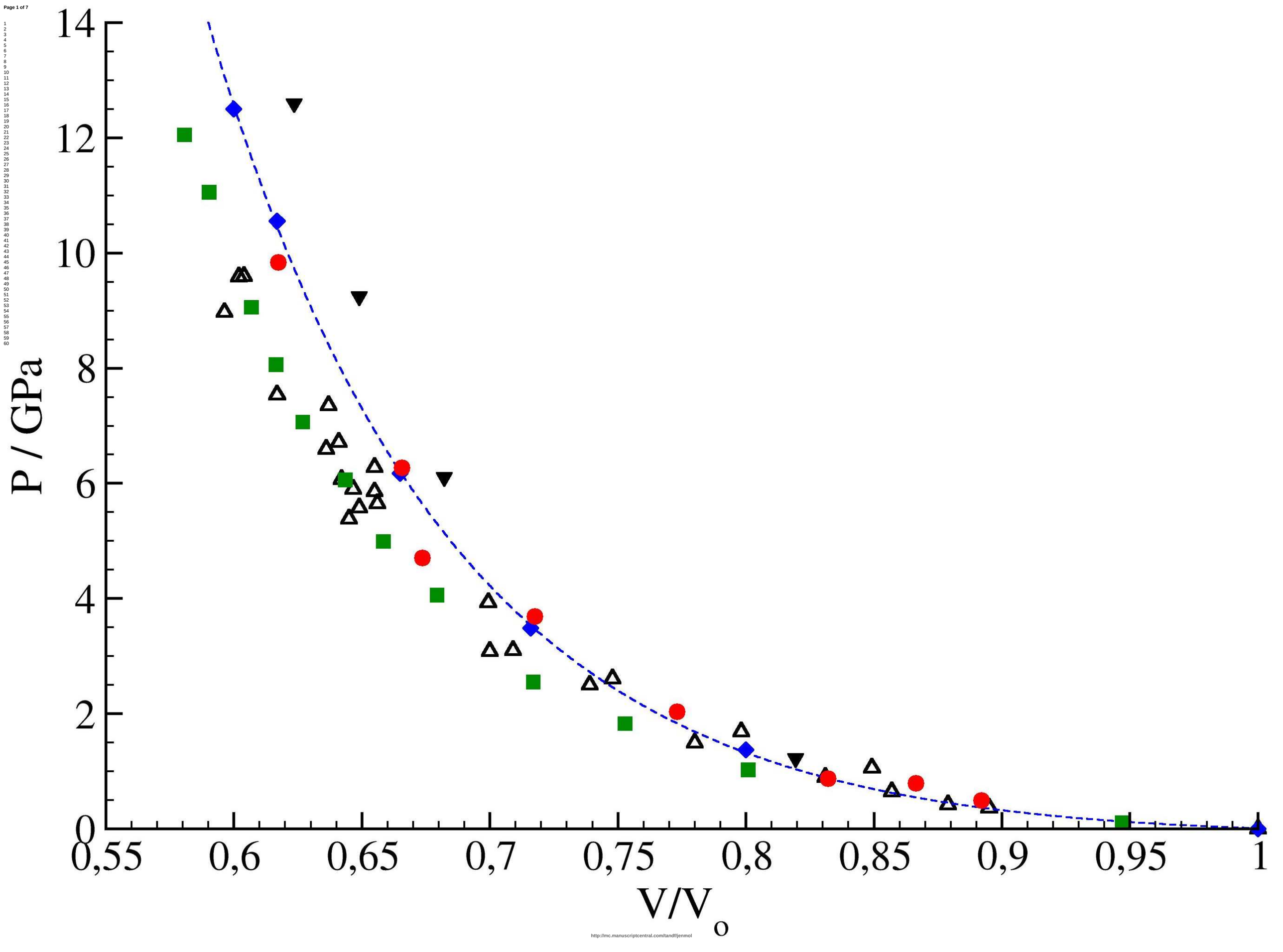
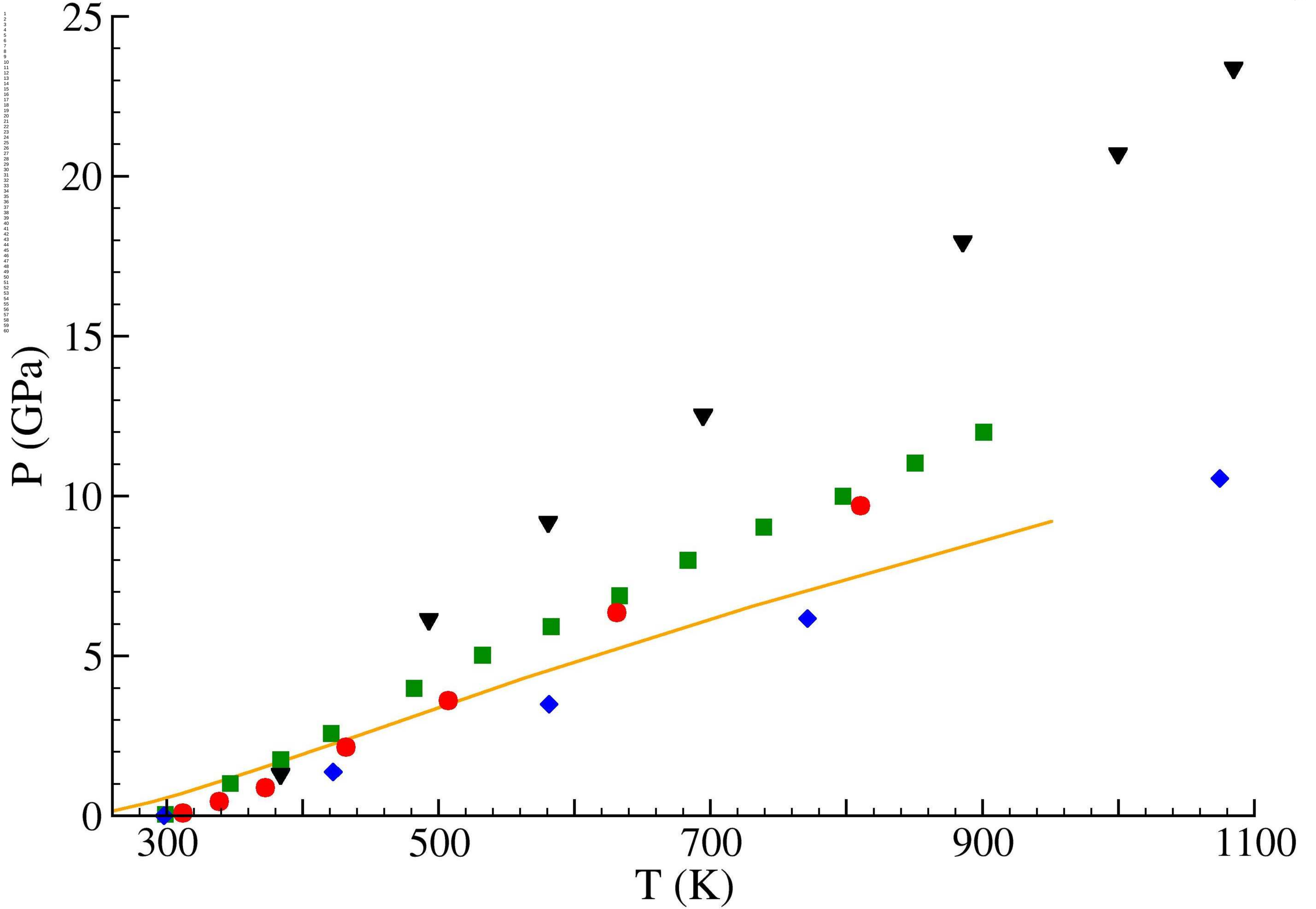
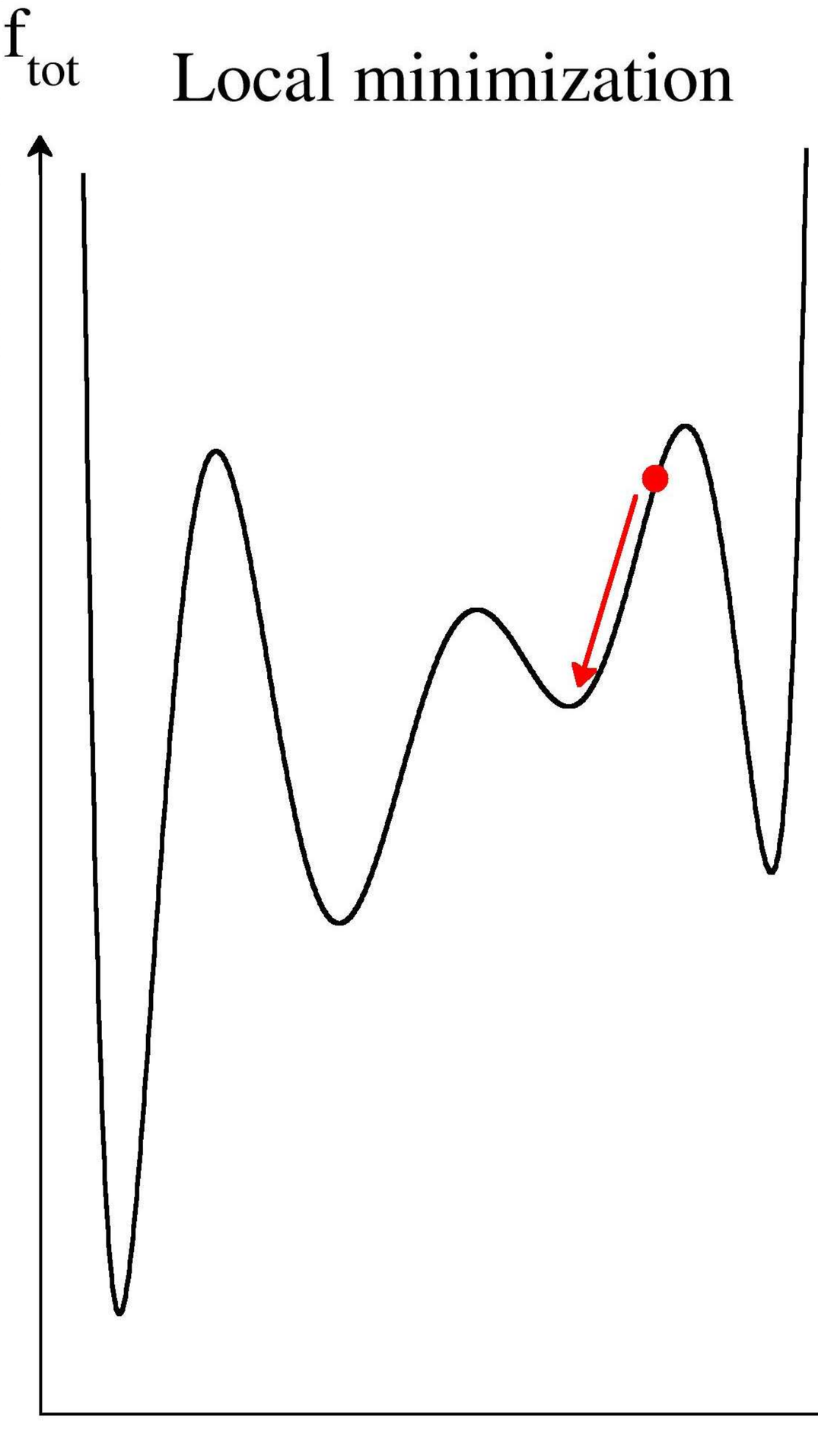
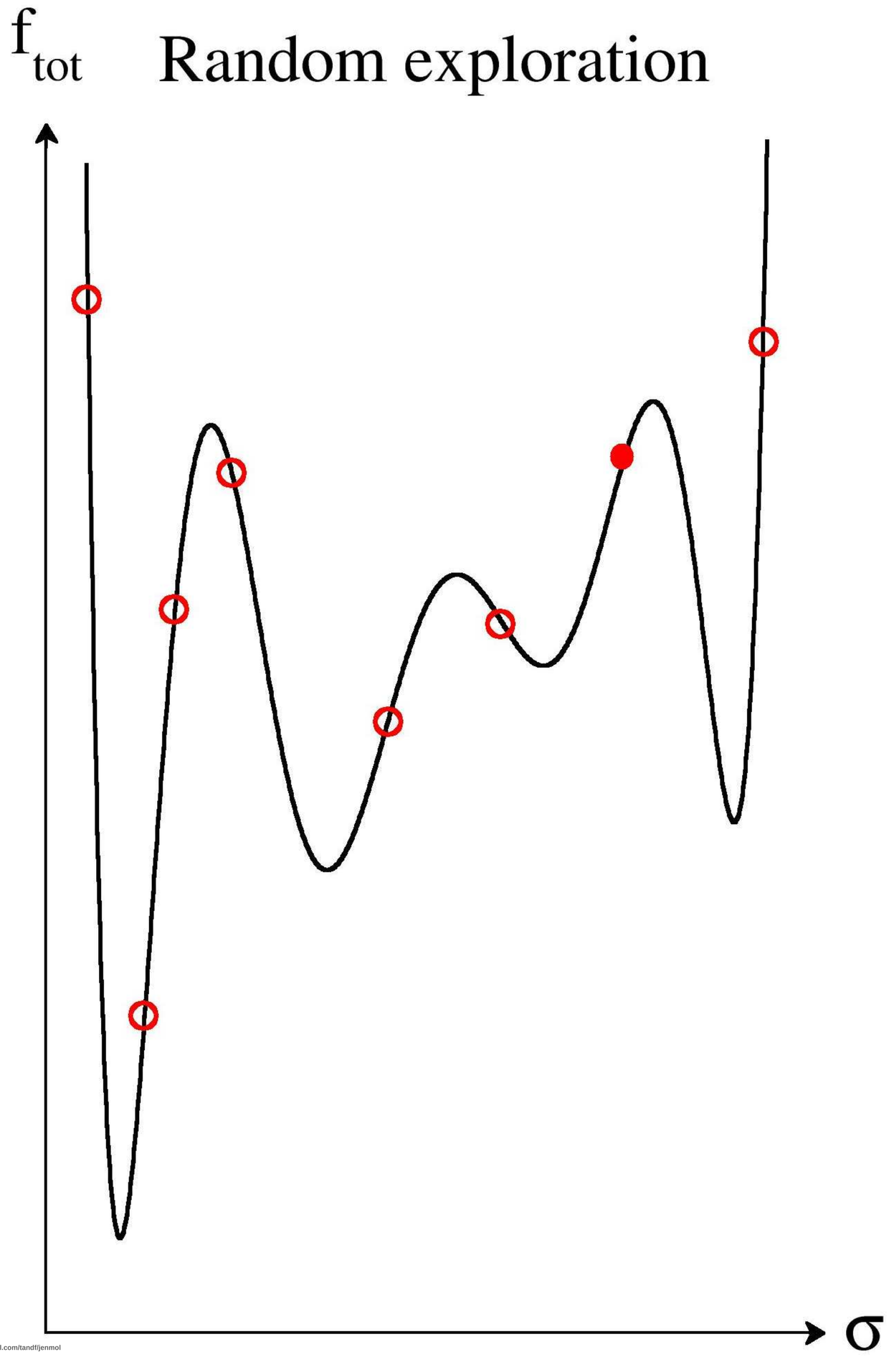
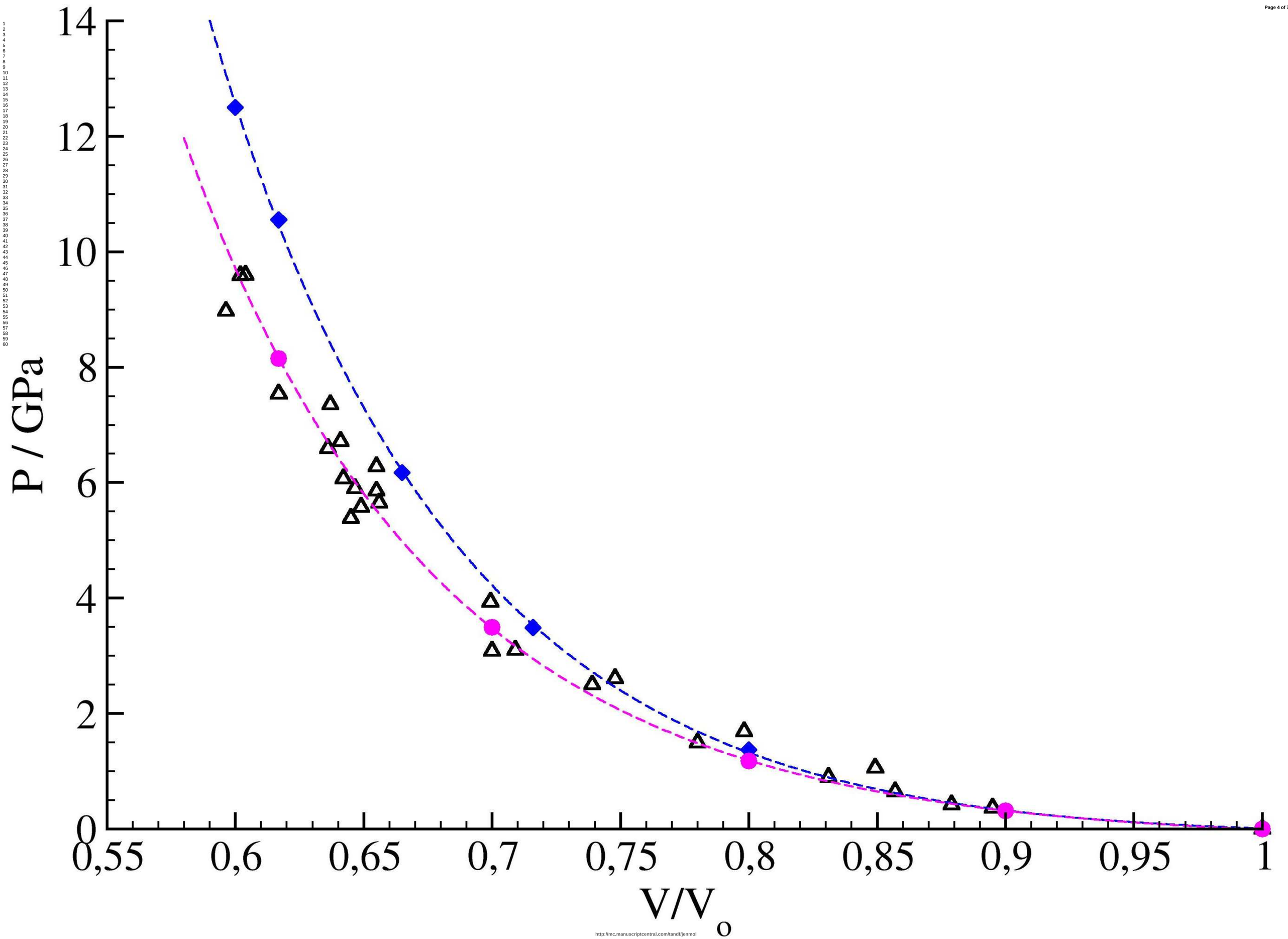
biblio.bib introduction.tex methods.tex results.tex conclusion.tex phjcp_mod.bst	

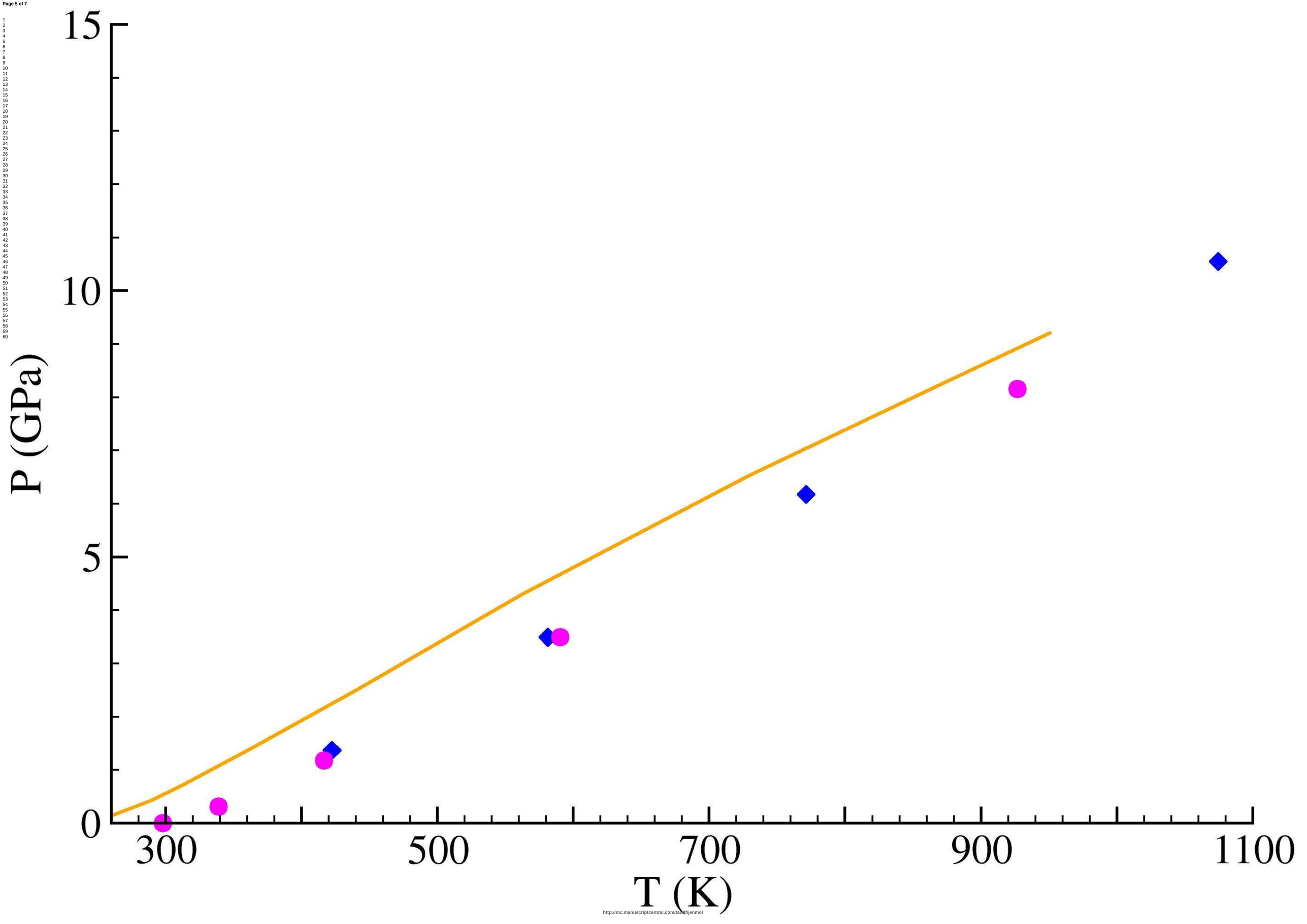

14
12
10
8
6
4
2
0
P / GPa
0,55
0,6
0,65
0,7
0,75
0,8
0,85
0,9
0,95
1
V/V
o

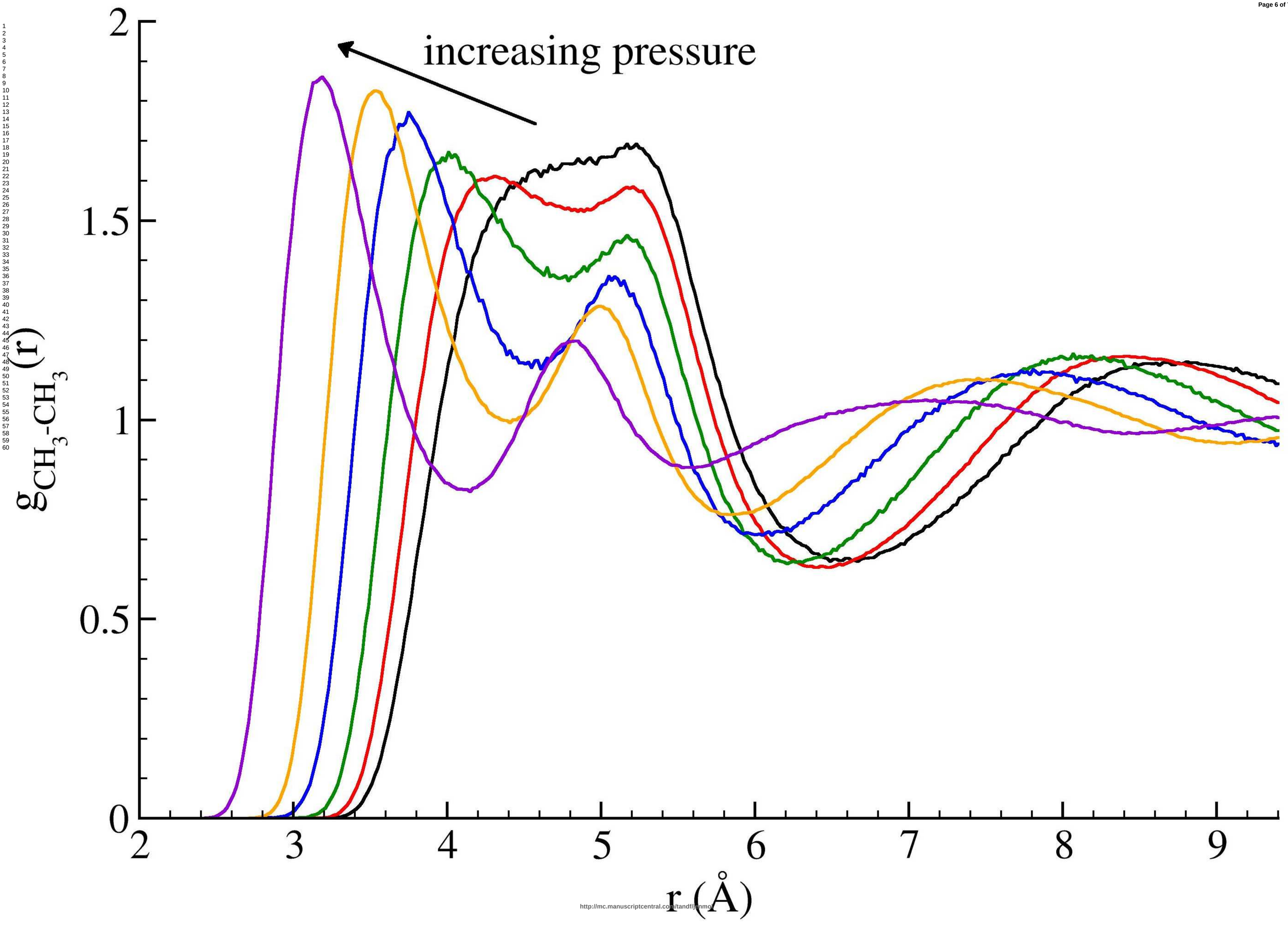

25
20
15
10
5
0
P (GPa)
300
500
700
900
1100
T (K)


f tot
Local minimization
σ


f tot
Random exploration
σ


P / GPa
0
2
4
6
8
10
12
14
0,55
0,6
0,65
0,7
0,75
0,8
0,85
0,9
0,95
1
V/V
o


15
10
5
0
P (GPa)
300
500
700
900
1100
T (K)


increasing pressure
$g_{CH_3\text{-}CH_3}(r)$
r (Å)
0
0.5
1
1.5
2
2
3
4
5
6
7
8
9